Science for Solutions, LLC

6211 Kaitlyn Court, West Windsor, NJ 08550   Ph & Fx: (609)275-7234

Terry Richard Stouch, PhD, President   tstouch@gmail.com

18 September 2016

David Mobley   John Chodera
Department of Pharmaceutical Sciences   Assistant Member
147 Bison Modular   Memorial Sloan-Kettering Cancer Center
University of California, Irvine   1275 York Ave., Box 357
Irvine, CA 92697   New York, NY 10065
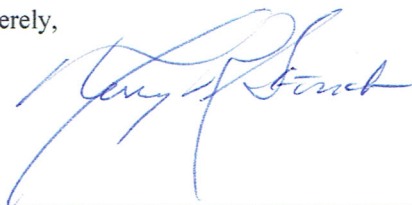
Dear Professors Mobley and Chodera:

I'm writing as Senior Editor-in-Chief of the *Journal of Computer Aided Molecular Design* (JCAMD) to express my continued enthusiasm for the SAMPL blind prediction challenge and my support for your plans to continue and expand the challenge via the proposed work, "Advancing predictive physical modeling through focused development of model systems to drive new modeling innovations." Previous SAMPL challenges have provided real benefit to the physical modeling community and have taught us a great deal of relevance to methods for predicting protein-ligand binding, as evidenced by the ongoing interest of pharmaceutical companies in these events. I am convinced your proposed work will do the same.

As you are aware, JCAMD has in the past supported the most recent 4 of the 5 SAMPL challenges by publishing special issues which focus on each iteration and the results of the challenge. For example, we are currently completing construction of the SAMPL5 special issue. Also, as long as SAMPL challenges continue to provide such important insight, this letter also serves to express my willingness to continue to publish SAMPL special issues. Participants would, as they have in the past, submit their papers by a specified deadline timely to the presentation of the results of the Challenge, and we would coordinate reviews and then publication in JCAMD, assuming the work is technically sound.

Previous JCAMD special issues on SAMPL have been well received, well cited, and a substantial service to the field. As one indication, the top ten SAMPL publications have already all been cited more than 50 and as many as over 80 times, per Google Scholar.

I look forward to our continuing our collaboration on the SAMPL challenges.

Sincerely,

Terry Richard Stouch, PhD
Senior Editor-in-Chief, Journal of Computer-Aided Molecular Design, Springer Publishing
President, Science for Solutions, LLC
    Consulting: Pharmaceutical Research: Drug Design, Discovery, Technologies, Process, Due Diligence; Computational Sciences; Chemistry, Biochemistry, Biophysics
American Chemical Society, Division of Computers in Chemistry, past Chair
University of Maryland, Baltimore, Affiliate Professor, Department of Pharmaceutical Sciences
Duquesne University, Adjunct Professor Department of Chemistry and Biochemistry, Bayer School of Natural and Environmental Sciences
American Association for the Advancement of Science (AAAS), Fellow
International Union of Pure and Applied Chemistry (IUPAC), Fellow

Springer